Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

N 1s core-level binding energies in nitrogen-doped carbon nanotubes: a combined experimental and theoretical study

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TABLE SI. Calculated N 1s core-level binding energy (in eV), obtained within Koopman's theorem approach, for the simplified N-doped carbon structure shown in Fig. S4. We consider the PBE exchange-correlation functional and different basis sets as specified in the first column.

Basis set	CLBE (Koopman)
6-31g*	378.52
6-311g**	378.32
Aug-cc-PVTZ	378.55

TABLE SII. Calculated N 1s core-level binding energy (in eV), obtained within Koopman's theorem approach, for the simplified N-doped carbon structure shown in Fig. S4. We consider the Aug-cc-PVTZ basis set and different exchange-correlation functionals as specified in the first column.

Exchange-correlation functional	CLBE (Koopman)
Perdew-Burke-Ernzerhof	378.55
Perdew-Wang 91	378.88
Becke-Lee-Yang-Parr	378.97

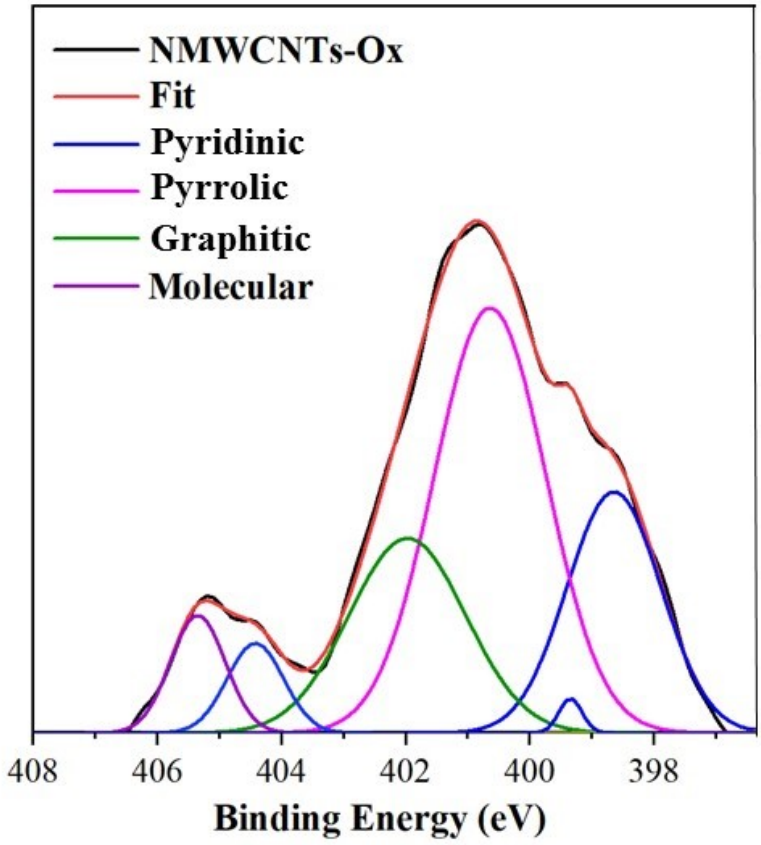

Figure S1. High-resolution XPS spectra for the N 1s signal (black line). The red curve corresponds to the fit. An additional small Gaussian function at 399.35 eV has been added which allows for a better description of the experimental signal around that energy domain. However, this small contribution does not alter the location neither the value of the integral below each one of the rest of the Gaussian curves, a fact that maintains the main conclusions of our work.

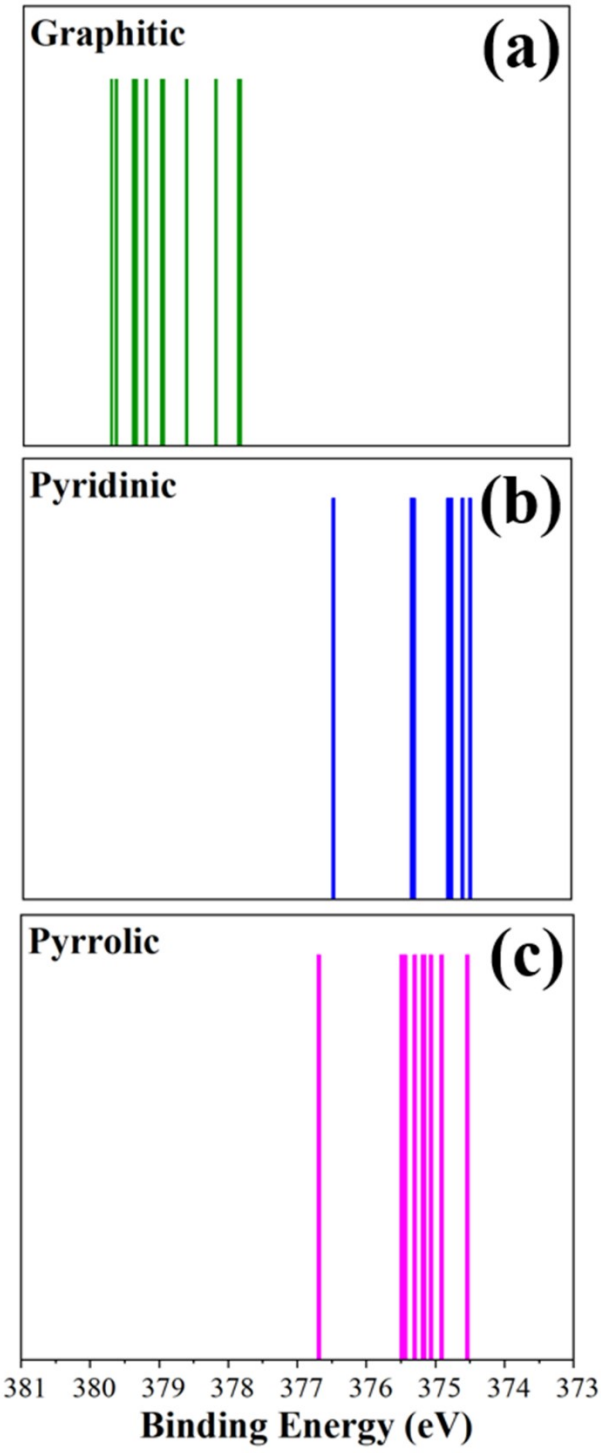

Figure S2. Simulated N 1s core-level binding energies, specified as vertical lines, for model N-doped CNTs (with oxygen free surfaces) having (a) graphitic, (b) pyridinic, and (c) pyrrolic nitrogen inclusions as specified in Figs. 1—6.

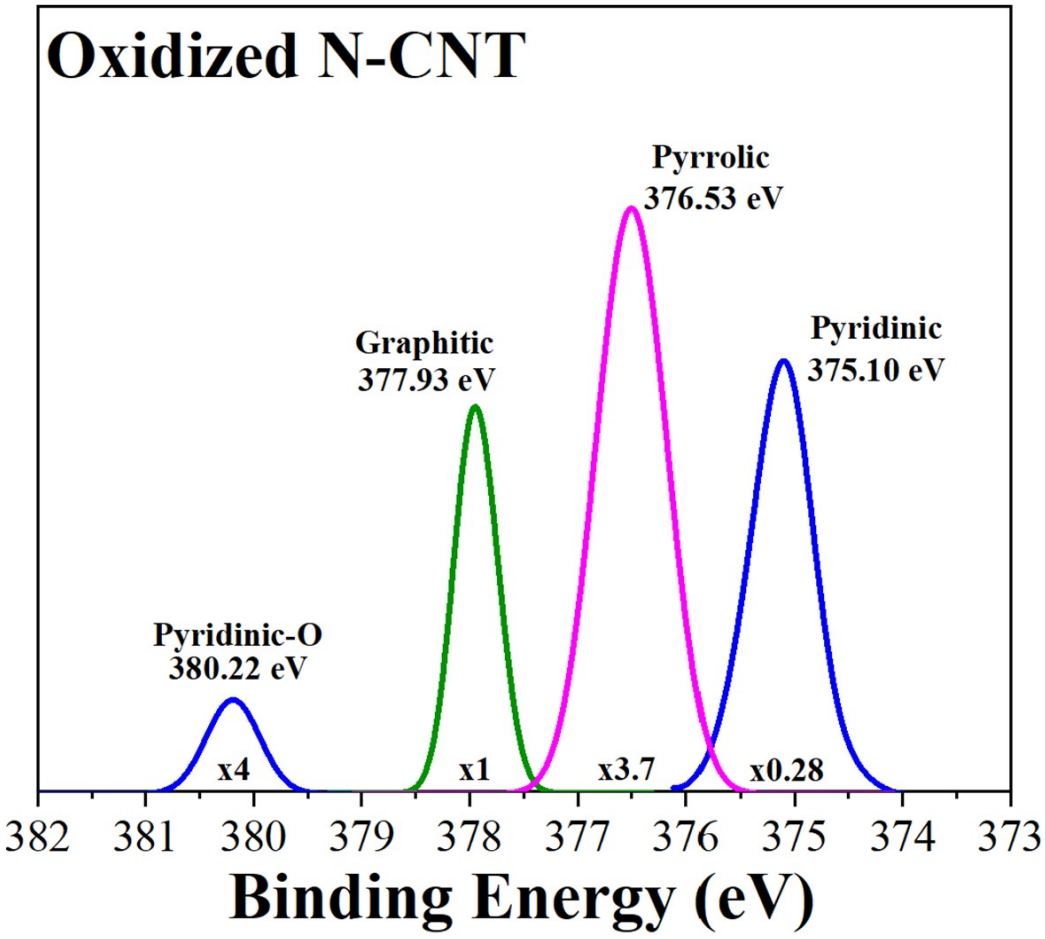

Figure S3. Simulated high-resolution N 1s spectra obtained by combining the selected Gaussian peaks associated to each one of the discrete distribution of CLBEs presented in Fig. 12 (see text).

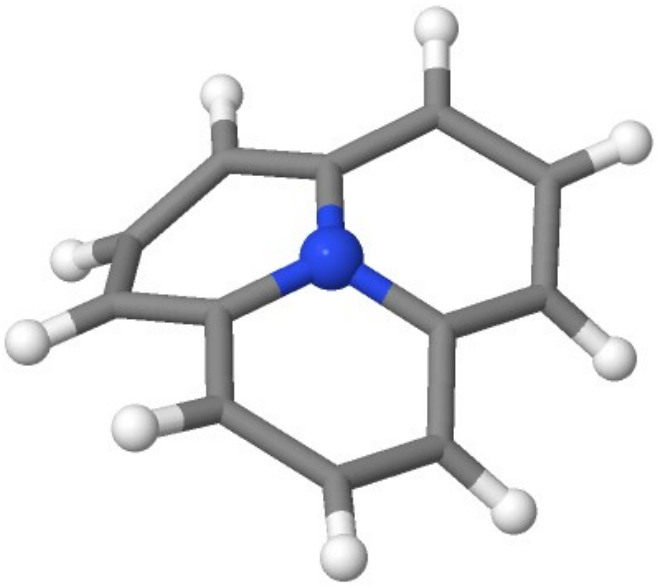

Figure S4. Small carbon fragment made of the N-doped CNT with a graphitic defect [see Fig. 5(a)] having a total number of 22 atoms.

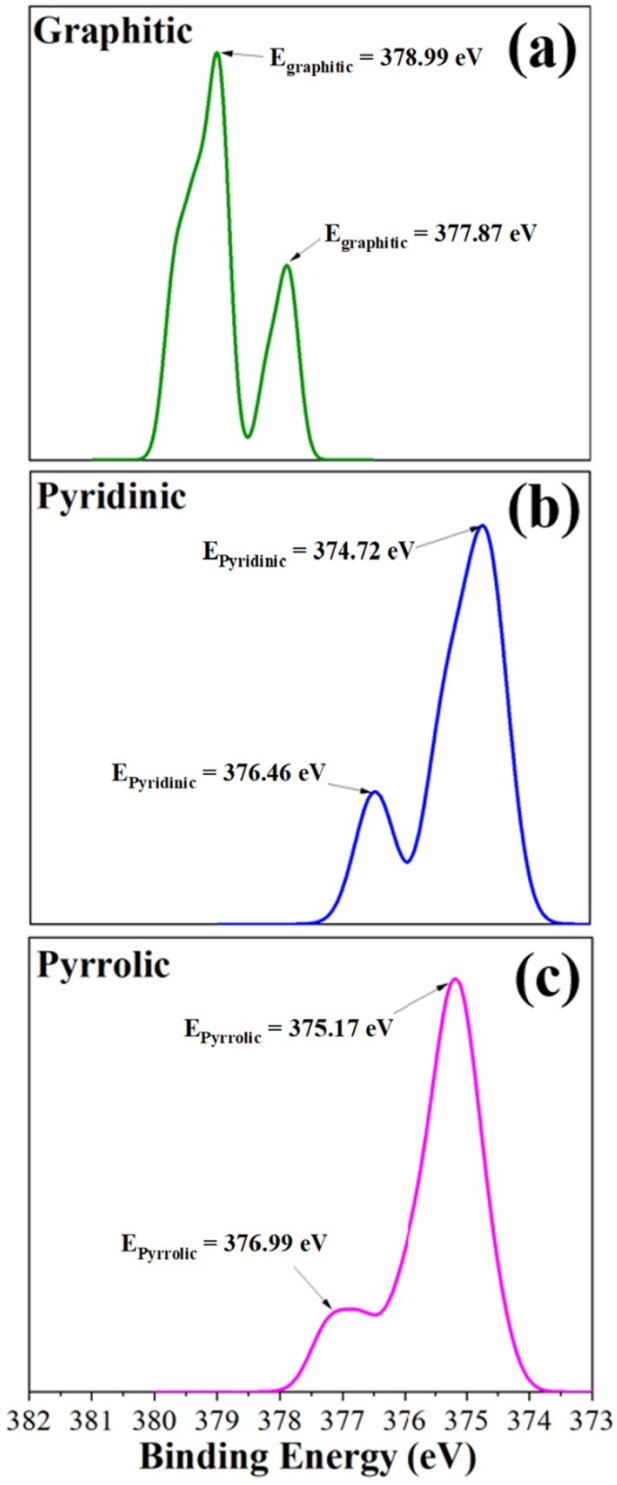

Figure S5. Simulated high-resolution N 1s spectra obtained by a Gaussian broadening of the discrete distribution of CLBEs presented in Fig. S2.

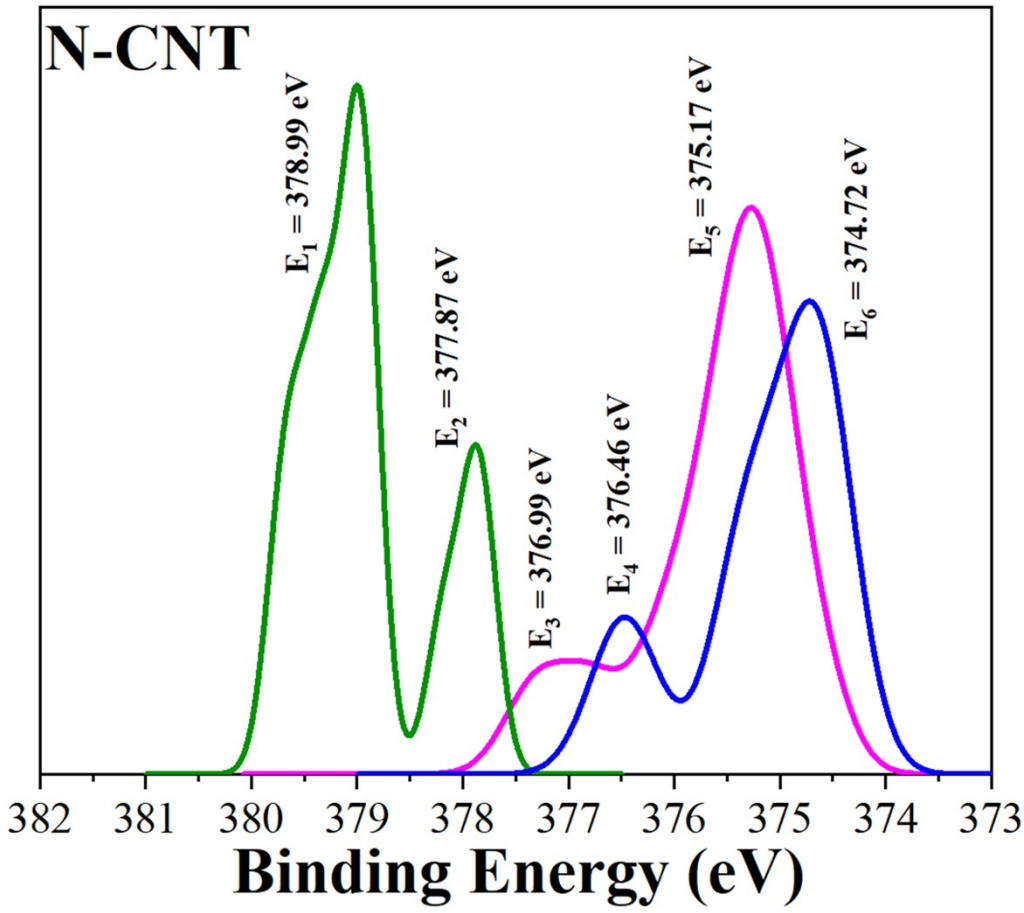

Figure S6. Simulated high-resolution N 1s spectra obtained by combining the Gaussian peaks associated to each one of the discrete distribution of CLBEs presented in Fig. S5.